$Si\text{-}Si_{1-x}Ge_x$ *n*-type resonant tunnel structures

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We report the first study of *n*-type $Si\text{-}Si_{1-x}Ge_x$ resonant tunnel structures. Strain effects in these structures induce splittings of the sixfold conduction bands into twofold and fourfold states, and change the band-edge profiles considerably. We demonstrate that resonant tunneling due to twofold, fourfold, or twofold and fourfold electrons can be selectively achieved by a proper choice of the layer thicknesses and alloy concentrations in the barrier layers. The possibilities for using these phenomena for making electron filters and making accurate determinations of the band offsets are discussed.

The capability of fabricating epitaxial $Si\text{-}Si_{1-x}Ge_x$ heterostructures by molecular beam epitaxy (MBE) has generated a great deal of interest in novel $Si\text{-}Si_{1-x}Ge_x$ based devices. Interesting properties such as strain-induced lowering of the alloy band gap,[1] modulation doping effect,[2] and a possible increase in optical absorption[3,4] have given $Si\text{-}Si_{1-x}Ge_x$ epitaxial structures an important place in semiconductor device research.[5,6] In this letter, we propose and theoretically analyze some novel properties of *n*-type $Si\text{-}Si_{1-x}Ge_x$ double-barrier structures. The main differences between these structures and III-V double-barrier structures occur because of the strain-induced splitting of the degeneracy in the lowest conduction band. In coherently strained $Si\text{-}Si_{1-x}Ge_x$ structures (grown in the [100] direction) with $x<0.85$, the sixfold degenerate conduction valley splits into four degenerate in-plane valleys and two degenerate out-of-plane valleys.[7] This offers the possibility of selectively tailoring the transport properties of the twofold or fourfold electrons. Here we analyze three interesting situations where twofold, fourfold, and combined twofold and fourfold resonant tunneling can be achieved selectively by proper choices of the layer thicknesses and alloy concentrations in the barrier layers.

An important application of *n*-type double heterostructures would be to investigate the relative band alignments of strained $Si\text{-}Si_{1-x}Ge_x$ epitaxial layers. The conduction-band offset would determine the positions of the resonant levels for the $Si_{1-x}Ge_x$ structures. Thus, experimental investigation of the low-temperature resonance peaks in the *I-V* curves could give us valuable information about the conduction-band offsets. Another application for these *n*-type resonant tunneling devices would be as electron filters that could be used to separate the fourfold and twofold electrons. Since the perpendicular transport properties of the fourfold electrons are significantly superior to those of the twofold electrons, an *n*-type resonant tunneling device operating at resonance could be used as an input stage to a majority-carrier device to enhance its performance. These devices could also be easily integrated into existing Si devices making novel devices possible such as double barrier/vertical field-effect transistors (DB/VFETs)[8] and double barrier/metal-semiconductor field-effect transistors (DB/MESFETs)[9] which have controllable negative differential resistance characteristics.

The structures we consider are engineered to cover three interesting cases. In the first case, we consider resonant tunneling of twofold electrons with nonresonant fourfold electrons. In the second case we consider resonant tunneling of fourfold electrons with nonresonant twofold electrons. In the third case we analyze a structure in which resonant tunneling from twofold or fourfold electrons can be selectively achieved by only a small change in the applied bias.

The calculation of the *I-V* curves for *n*-type $Si\text{-}Si_{1-x}Ge_x$ epitaxial structures is carried out within the envelope function formalism.[10] In a typical calculation, we first calculate the screening (band bending) in the cladding layers and the potential drops in the well region based on the Thomas–Fermi model. We then calculate the complex band structure of the $Si_{1-x}Ge_x$ layers to describe the decay of the twofold and the fourfold conduction electrons in the barrier regions.[4,11] We next use the transfer matrix method, and the decay lengths given by the local complex band structure to construct the envelope wave functions describing the tunneling states. Finally, we sum the contribution to the current from the Fermi distribution of electrons in each electrode, to obtain the total current. Further details of the band structure calculations are given elsewhere.[4,12]

The strain distribution in the epilayers is calculated assuming that the layers become elastically deformed to assume the in-plane lattice constant set by the substrate. This assumption should be valid for the structures considered here, since they have layer thicknesses less than the critical thicknesses given by Matthews and Blakeslee.[13]

The self-consistent *ab initio* calculations of Van de Walle and Martin[14] suggest that the average valence-band offset between Si and Ge depends very little on strain, and has a value $\Delta E_V \approx 0.54$ eV. We have used this result and the phenomenological deformation potential model of Kleiner and Roth[15] to calculate the strain dependence of the $Si\text{-}Si_{1-x}Ge_x$ conduction bands. Our results are in close agreement with the earlier work of People and Bean.[16,17] Further details on the strain dependence of the conduction-band offsets are given elsewhere.[18]

Since the fourfold conduction-band minima have $k_\parallel \neq 0$ and the twofold minima have $k_\parallel = 0$, we expect very little interaction between the twofold and the fourfold contributions to the current ($k_\parallel$ is conserved across heterojunction interfaces). This allows independent treatment of the two-

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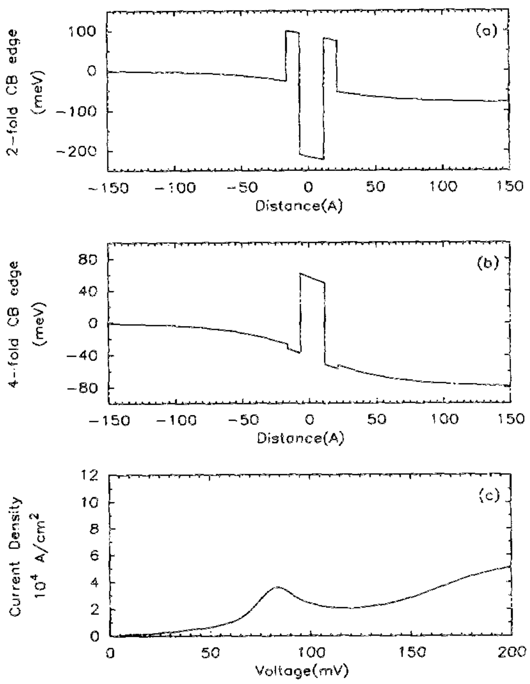

FIG. 1. Band diagram for a structure exhibiting resonant tunneling of twofold electrons and nonresonant fourfold electrons. The potential seen by the twofold and fourfold electrons is shown in (a) and (b), respectively. The bias is chosen to correspond to the peak in the J-V curve of (c).

fold and the fourfold current. The current due to the fourfold valleys should be larger than the twofold current for the same band alignment because of the lower effective masses perpendicular to the layers. Specifically, for an electron distribution with the same Fermi energy, we find that the contribution to the total current after integration over the density of states varies as $(m_\perp^*)^{-1/2}$, where $m_\perp^*$ is the effective mass perpendicular to the barrier layers. All calculations are done assuming an electron distribution at 4.2 K in the electrodes.

The first of the three devices we consider is an n-type double-barrier structure where resonant tunneling by the twofold electrons is achieved while the fourfold electrons exhibit a nonresonant single-barrier behavior. Since a double barrier at resonance has a transmission coefficient close to unity, this device can be thought of as an electron filter that passes twofold electrons and blocks the fourfold electrons. The structure of this device is shown in Fig. 1. The motivation behind this device was to study a case where we can obtain resonant tunneling behavior from the twofold minima, giving us information about the magnitudes of the strain split twofold band offset. The structure is a symmetric one which consists of strain relaxed and degenerately doped (10^{18} cm^{-3}) n-type $Si_{0.6}Ge_{0.4}$ cladding layers. The barriers are chosen to be 10 Å layers of $Si_{0.4}Ge_{0.6}$ on each side, and the well region is chosen to be an 18 Å layer of Si. In this device the twofold electrons are subjected to a double-barrier structure with a barrier height of ≈ 130 meV. We have intentionally lowered the twofold conduction-band minima in the well layer to achieve a single-barrier profile for the fourfold electrons. The typical band diagram near the occurrence of the peak in the J-V curve (at ≈ 80 meV bias) is shown in Figs. 1(a) and 1(b) as seen by the twofold and the fourfold electrons, respectively. In Fig. 1(c) we show the J-V curve corresponding to this structure. There is a weak resonance peak associated with the resonant tunneling current from the twofold electrons. This peak is associated with the second resonance in the well. The peak-to-valley ratios obtained are fairly small due to the thinness of the barriers used, and the small value of the band offset. There is also a large nonresonant current from the fourfold electrons contributing to the total current.

The second device we studied exhibits resonant tunneling by the fourfold electrons, and nonresonant tunneling by the twofold electrons. A device such as this can be used to study the behavior of the strain-split fourfold band offset. In contrast to the earlier device, this device can be thought of as an electron filter that passes fourfold electrons and blocks all twofold electrons. The band profiles for this device are shown in Fig. 2. The layer thicknesses and the alloy concentrations are fairly similar to those of the structure in Fig. 1. This structure consists of strain relaxed and degenerately doped (10^{18} cm^{-3}) n-type $Si_{0.6}Ge_{0.4}$ cladding layers. The barriers are chosen to be 10 Å layers of Si on each side, and the well region is chosen to be an 18 Å layer of $Si_{0.4}Ge_{0.6}$. In Fig. 2(c) we show the J-V curve corresponding to this structure. In this structure we see that the fourfold electrons are subjected to a double-barrier structure with a barrier height of 100 meV. We have intentionally lowered the fourfold conduction-band minima in the well layer in order to achieve a single-barrier profile for the twofold electrons. The typical band diagram near the occurrence of the resonance (at ≈ 75

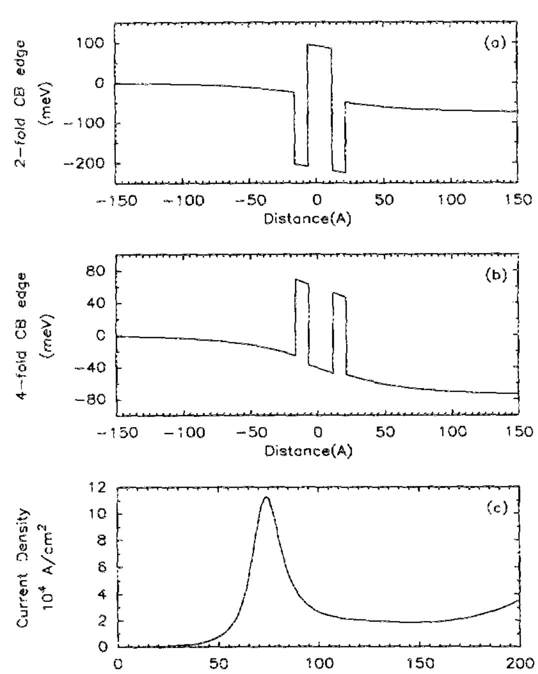

FIG. 2. Band diagram for a structure exhibiting resonant tunneling of fourfold electrons and nonresonant twofold electrons. The potential seen by the twofold and fourfold electrons is shown in (a) and (b), respectively. The bias is chosen to correspond to the peak in the J-V curve of (c).

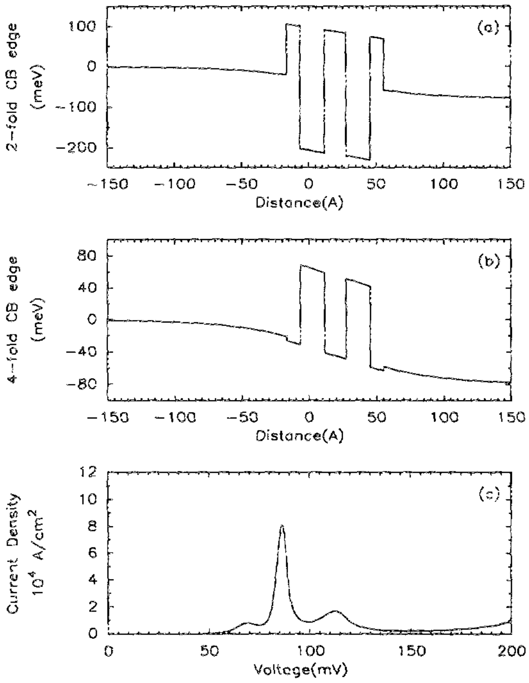

FIG. 3. Band diagram for a structure exhibiting resonant tunneling of twofold or fourfold electrons, depending on the biasing conditions. The twofold electrons are subjected to a triple-barrier potential while the fourfold electrons are subjected to a double-barrier potential. The bigger peak in the *J-V* curve is due to fourfold resonant tunneling, while the smaller peaks are due to the twofold resonant tunneling. The bias chosen in (a) and (b) corresponds to the fourfold peak in the *J-V* curve of (c).

meV) is shown in Figs. 2(a) and 2(b). The *J-V* curve shows a resonance peak associated with the resonant tunneling current from the fourfold electrons.

The third device we consider has the feature of exhibiting resonant tunneling from twofold and fourfold electrons at different applied voltages. The advantage of such a device is that by controlling the applied bias, we can control the ratio of twofold to fourfold electrons that is transmitted. The band profiles for this device are shown in Fig. 3. This is a $Si\text{-}Si_{1-x}Ge_x$ structure with two well regions and three barrier regions seen by the twofold electrons and a regular double-barrier structure seen by the fourfold electrons. The cladding layers are strain relaxed *n*-type $Si_{0.6}Ge_{0.4}$ (10^{18} cm^{-3}). The three-barrier layers are $Si_{0.4}Ge_{0.6}$ and the two-well layers are Si. This triple-barrier structure was chosen because a band alignment that would give favorable resonant tunneling amplitudes for the twofold and the fourfold electrons simultaneously could not be found within the simple double-barrier geometry. In Figs. 3(a) and 3(b) we show schematic illustrations of the band-edge profile seen by the twofold and the fourfold electrons. The biasing condition shown in Figs. 3(a) and 3(b) is in the proximity of the fourfold peak in the *J-V* curve (*c*) (≈ 80 meV). The peaks shown in the *J-V* curves of Fig. 3(c) corresponding to this structure can be attributed to two resonances associated with the twofold electrons and a single resonance due to the fourfold electrons. The biggest peak in the *J-V* curve is due to the fourfold resonance, while the two smaller peaks are due to the twofold resonances.

In this letter we have analyzed *J-V* curves associated with $Si\text{-}Si_{1-x}Ge_x$ *n*-type resonant tunneling devices. The predictions made in this letter are based on the phenomenological deformation potential theory and the assumed value of the valence-band offset for the Si/Ge system which is an input parameter. The presence of resonant tunneling from the twofold and fourfold electrons will depend strongly on the actual conduction-band offsets. Thus, the study of these *n*-type Si/Ge devices would provide valuable information about the relative alignments of the conduction bands. The novel *n*-type devices discussed in this letter show great promise as electron filters for separating degenerate Si electrons into twofold and fourfold components. Thus, these devices can be utilized to enhance the quality of Si-based majority-carrier devices by isolating the fourfold electrons which have higher mobility for transport in the direction of the applied field. The integration of *n*-type $Si\text{-}Si_{1-x}Ge_x$ double-barrier structures with existing Si devices may allow the realization of many novel and interesting semiconductor devices.

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